degree of attraction and in angular width of the interaction. Comparison with homologous and mutant versions of the model protein also identifies a key force in crystal contact formation: the presence of high-entropy residues significantly destabilizes the crystal interface.
In order to further study the crystallization dynamics, we represent proteins with a Kern-Frenkel patchy particle model with an additional torsion potential: the patch geometry, the range of interaction and the width of the patches are determined using the data from the molecular dynamics simulations. Using Monte Carlo techniques, we trace the phase diagram and crystallization pathway of the different proteins under study. The results suggest new strategies for protein crystallization.

1361-Pos Board B131
Effects of Macromolecular Crowding on the Assembly of Self-Associating Particles: Implications to Nuclear Compartmentalization
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Crowded nature of biological cells has profound influences on cellular structure and function, and its importance in nuclear compartmentalization has been suggested in recent experiments. Using computer simulations of a simple physical model, we investigated the phase behavior of self-associating particles in the presence of crowding agents, as a model to study crowding effects on the nuclear compartmentalization. We show that the phase diagram of self-associating particles is altered significantly due to crowding and the extent of such crowding effect is affected when interactions between self-associating particles and crowding agents are considered. We conclude that the presence of non-attractive crowding agents with volume exclusion interactions plays an important role in the formation and maintenance of nuclear compartments.

1362-Pos Board B132
Nanofluidic Studies of DNA Compaction by Macromolecular Crowding and Architectural Protein
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The study of single DNA molecules confined in a nanochannel is of importance from both biotechnological and biophysical points of view. We produce nanochannels in cheap PDMS based biochips. The two-dimensional cross-sectional diameter of the channels is in the range of 50 to 300 nm. We measure the extensions of single bacteriophage DNA molecules in various environmental conditions with fluorescence microscopy. In this contribution, two important and related issues will be addressed. The first issue is the control of conformation of DNA by macromolecular crowding. We have investigated dextran and the like-charge proteins bovine serum albumin (BSA) and hemoglobin (Hb). As a surprising result, we found that the DNA molecules take a more extended rather than a more compacted conformation in the presence of low volume fractions of dextran. At higher volume fractions, the DNA molecules collapse into a condensed state. DNA collapse was also observed for the like-charge proteins, albeit at much lower volume fractions as compared to dextran. The second issue is the effect of architectural protein. For this purpose, we have investigated the effects of the bacterial nucleoid associated H-NS and HU proteins. Our results show that the interplay of DNA/ligand interaction, osmotic pressure, like charge attraction, and anisotropic confinement is of paramount importance in controlling the conformation and compaction of DNA. The biochip provides a platform to investigate single biomolecules and is complementary to other single molecule techniques such as those based on molecular tweezers. Some other exemplary experiments on the structure and dynamics of single DNA molecules inside nanochannels, which are in progress in our laboratories, will be presented.

1363-Pos Board B133
Shaken, Not Stirred: Collapsing a Peptoid Monolayer to Produce Free-Floating, Stable Nanosheets
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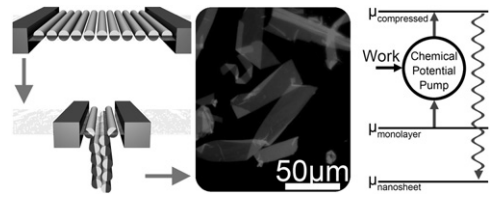
Two-dimensional nanomaterials play a critical role in biology (e.g., lipid bilayers) and electronics (e.g., graphene), but are difficult to directly synthesize with a high level of precision. Biomimetic peptoid nanosheet bilayers are a versatile synthetic platform for constructing multifunctional, precisely ordered two-dimensional nanostructures. Here we show that nanosheet formation occurs through an unusual monolayer intermediate at the air-water interface. Lateral compression of a self-assembled peptoid monolayer beyond a critical collapse pressure results in the irreversible production of nanosheets. An unusual thermodynamic cycle is employed on a preparative scale, where mechanical energy is used to buckle an intermediate monolayer into a more stable nanosheet. Detailed physical studies of the monolayer-compression mechanism revealed a simple preparative technique to produce nanosheets in 95% overall yield, by cyclical monolayer compressions in a rotating closed vial. Compression of monolayers into stable, free-floating products may be a general and preparative approach to access two-dimensional nanomaterials.



1364-Pos Board B134
Mechanism of Photo-Switching in mIrisGFP
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Fluorescent proteins (FPs) have become extremely valuable tools in the life sciences. Due to the latest advances in the light microscopy, there is a steady need for FPs with improved spectral properties. Directed engineering, however, requires a detailed knowledge of the interplay between chromophore and protein environment.
Here, we present an investigation of the pH- and light-driven interconversion reactions of the chromophore species in mIrisGFP. It is a monomeric fluorescent protein that can reversibly be switched between a bright green fluorescent and a dark state by illumination with light of specific wavelengths. Structurally, this photo-switching is based on a conformational change of the chromophore between a cis and a trans state. This isomerization reaction is accompanied by extensive rearrangements of chromophore pocket, which results in significant changes in the photo-physical properties of the chromophore isomers. Hence, several light-activated reaction pathways can be distinguished for exciting either the neutral or anionic and cis or trans chromophore. The individual reaction pathways are extensively intertwined because of the ground state equilibria. Consequently, the overall effect achieved with light of a particular wavelength is determined by the ratio of the rate coefficients and the relative probabilities to excite the reacting species. Further studies and engineering approaches to influence these parameters are ongoing.

1365-Pos Board B135
Direct Measurements of Electric Fields in Weak Hydrogen Bonds
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Hydrogen bonds are of fundamental importance for structure, function and dynamics in numerous chemical and biological systems. They vary enormously in bond energies from ~15-40 kcal/mol for the strongest interactions, to less than 4 kcal/mol for the weakest. It is proposed, largely based on calculations, that strong hydrogen bonds have more covalent character, whereas electrostatics are more important for weak hydrogen bonds, but the precise contribution of electrostatics to hydrogen bonding is widely debated. Our strategy is to select interacting pairs of molecules in which one partner displays a vibrational mode whose vibrational Stark tuning rate can be measured, then study vibrational shifts with different partners. The analysis is made quantitative by comparison with electric fields calculated with DFT methods in the gas-phase. The combination of vibrational Stark effect measurements of electric fields and high-level quantum chemistry calculations is a general strategy for quantifying and characterizing the origins of intermolecular interactions.

1366-Pos Board B136
Entropic Modulation of Ion Transport through OmpF Channel. Molecular Basis of pH Sensing Derived from Cooperative Interactions
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Porins are channel-forming proteins that are located in the outer membranes of Gram-negative bacteria and allow the influx of hydrophilic nutrients and the extrusion of waste products. The inactivation of these wide channels is thought to play an important role in the survival of the bacteria in acidic media. We investigate here the mechanism responsible for pH sensing in the trimeric porin OmpF, of E. coli. Planar lipid bilayer electrophysiology was used to study the effect of pH on the transport properties of the OmpF channel in its fully open, ''nongated'' conformation. At low pH we observe a drastic drop in the OmpF open channel conductance that is accompanied by a huge increase of the current noise and inversion of the channel selectivity. All these channel features are strongly dependent on the salt concentration and, according to the Hill